Connections between Single body and Many body Models for Moiré Materials

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Mathematical Aspects of 2D Quantum Materials and Meta-materials
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Outline

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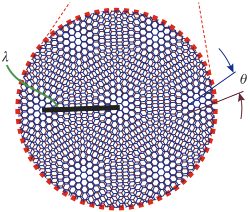
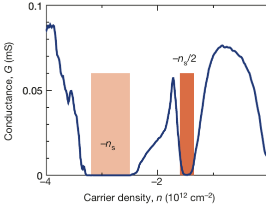
Twisted bilayer graphene as a correlated insulator





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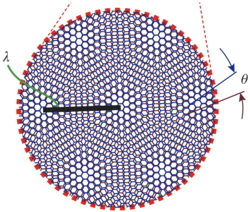

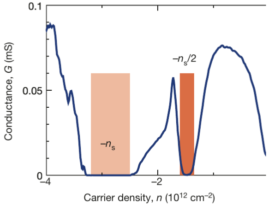

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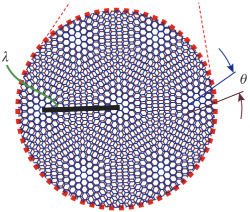

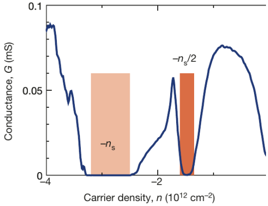

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- Nature of electron correlation?

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- BM model is a non-interacting model and always predicts zero band gap due to symmetries. So insulating phase must be due to electron-electron interactions.
- Hartree-Fock theory is the simplest theory describing electron-electron interactions.
- Can Hartree-Fock theory describe the correlated insulating phase?

(Kang, Vafek, PRL 2019), (Bultinck et al, PRX 2020), (Liu et al, PRR 2021), (Bernevig et al, PRB 2021)

Chiral Hamiltonian for TBG (spinless, valleyless)

- Chiral BM Hamiltonian[1]; $\alpha \propto \theta^{-1}$

$$H(\alpha) = \begin{bmatrix} 0 & D(\alpha)^\dagger \\ D(\alpha) & 0 \end{bmatrix}$$

with $D(\alpha) = \begin{bmatrix} D_{x_1} + iD_{x_2} & \alpha U(\mathbf{r}) \\ \alpha U(-\mathbf{r}) & D_{x_1} + iD_{x_2} + i \end{bmatrix}$

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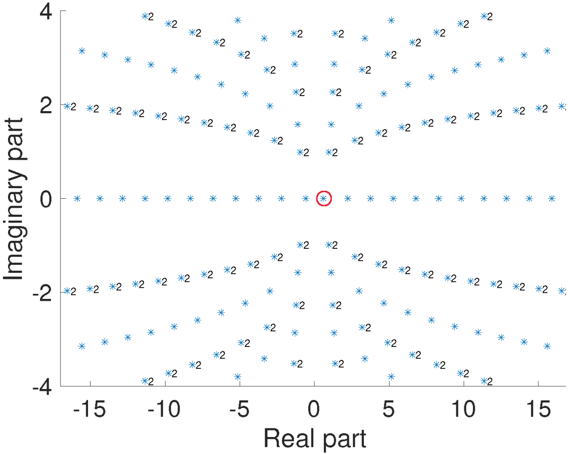
- For “magic” α, this model exhibits either 2 or 4 flat bands[2].

[1] (Tarnopolsky, Kruchkov, Vishwanath, PRL 2019),
[2] (Becker, Humbert, Zworski arXiv:2306.02909)

Magic angle and multiplicity of TBG

$M =$ multiplicity of magic angle α. * means $M = 1$.
$\#(\text{flat bands}) = 2M$.



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- $\hat{f}^\dagger_{m\mathbf{k}}, \hat{f}_{m\mathbf{k}}$: creation, annihilation operators associated with $\psi_{m\mathbf{k}}$.

Flat Band Interacting (FBI) Hamiltonian

$$\hat{H}_{FBI} := \frac{1}{N_{\mathbf{k}}|\mathbb{R}^2/\Gamma|} \sum_{\mathbf{q}' \in \mathcal{K}+\Gamma^*} \hat{V}(\mathbf{q}')\widehat{\rho}(\mathbf{q}')\widehat{\rho}(-\mathbf{q}')$$

$$\widehat{\rho}(\mathbf{q}') := \sum_{\mathbf{k}\in\mathcal{K}} \sum_{m,n\in\mathcal{N}} [\Lambda_{\mathbf{k}}(\mathbf{q}')]_{mn} \left(\hat{f}^{\dagger}_{m\mathbf{k}} \hat{f}_{n(\mathbf{k}+\mathbf{q}')} - \frac{1}{2}\delta_{mn}\delta_{\mathbf{q}'\in\Gamma^*} \right).$$

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  - $\Rightarrow$ $\hat{H}_{FBI}$ is non-commuting and frustration-free with long range interactions.

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Indices: in-layer position ($\mathbf{r}$); sublattice (σ); layer (j)

- Sublattice symmetry $\mathcal{Z}$

$$\mathcal{Z}u(\mathbf{r};\sigma,j) = \sigma u(\mathbf{r};\sigma,j)$$

- $C_{2z}\mathcal{T}$ symmetry $\mathcal{Q}$

$$\mathcal{Q}u(\mathbf{r};\sigma,j) = \overline{u(-\mathbf{r};-\sigma,j)}$$

- Layer symmetry $\mathcal{L}$

$$\mathcal{L}u(\mathbf{r};\sigma,j) = (-1)^j u(-\mathbf{r};\sigma,N-j)$$

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- These two blocks define the chiral sectors of TBG: $+$ and $-$.

Ferromagnetic Slater Determinants

Ferromagnetic Slater determinant (FSD) states fully fill one of the two chiral sectors (half filling)

$$|\Psi_+\rangle = \prod_{\mathbf{k}} \prod_{n>0} \hat{f}^\dagger_{n\mathbf{k}} |\text{vac}\rangle \qquad |\Psi_-\rangle = \prod_{\mathbf{k}} \prod_{n<0} \hat{f}^\dagger_{n\mathbf{k}} |\text{vac}\rangle$$

Theorem

With $\mathcal{Z}, \mathcal{Q}, \mathcal{L}$ symmetries, FSD states are many-body ground states of the FBI Hamiltonian for N-layer magic angle graphene.

(Becker, Lin, **KDS**, CMP 2025)

Our goal: characterize the entire

ground state manifold

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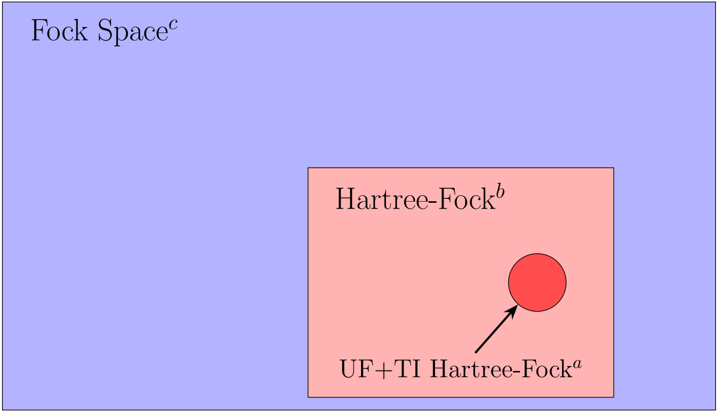
Hierarchy of Admissible States



UF = uniformly filled, TI = translation invariant.

[a](Becker, Lin, Stubbs CMP 2025), [b](Stubbs, Becker, Lin, SIAM MMS 2025), [c](Stubbs, Ragone, MacDonald, Lin, arXiv: 2503.20060)

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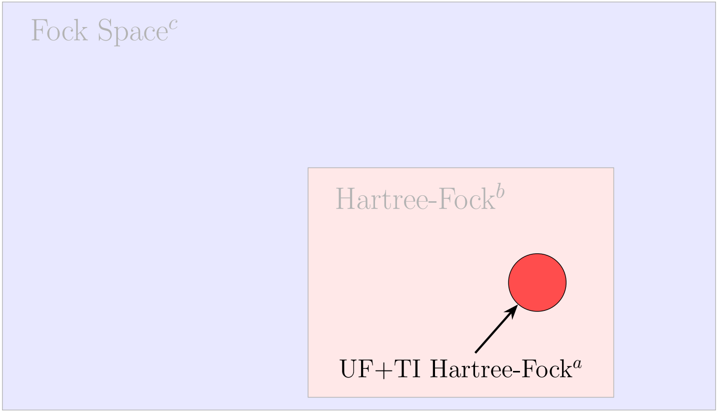

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Uniform Filling and Translation Invariance

- One body reduced density matrix (1-RDM) $[P(\mathbf{k},\mathbf{k}')]_{nm} = \langle\Psi|\hat{f}^{\dagger}_{m\mathbf{k}'}\hat{f}_{n\mathbf{k}}|\Psi\rangle$. $P^2 = P$.

$$P = \begin{bmatrix} P\left(\mathbf{k}_1,\mathbf{k}_1\right) & P\left(\mathbf{k}_1,\mathbf{k}_2\right) & \cdots & P\left(\mathbf{k}_1,\mathbf{k}_{N_\mathbf{k}}\right) \\ P\left(\mathbf{k}_2,\mathbf{k}_1\right) & P\left(\mathbf{k}_2,\mathbf{k}_2\right) & \cdots & P\left(\mathbf{k}_2,\mathbf{k}_{N_\mathbf{k}}\right) \\ \vdots & \vdots & \ddots & \vdots \\ P\left(\mathbf{k}_{N_\mathbf{k}},\mathbf{k}_1\right) & P\left(\mathbf{k}_{N_\mathbf{k}},\mathbf{k}_2\right) & \cdots & P\left(\mathbf{k}_{N_\mathbf{k}},\mathbf{k}_{N_\mathbf{k}}\right) \end{bmatrix}$$

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- Uniformly Filled + Translational Invariance

$$\mathrm{Tr}\left(P(\mathbf{k},\mathbf{k})\right) = \text{(constant)}$$

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Uniformly Filled, Translation Invariant Hartree-Fock

Theorem (Informal)

Under $\mathcal{Z}, \mathcal{Q}, \mathcal{L}$ symmetries and non-degeneracy assumptions, there are only two uniformly filled, translation invariant Hartree-Fock ground states.

Uniqueness for UF+TI Hartree-Fock

Theorem

Assume $\mathcal{K}$ is a sufficiently fine grid. If $\exists \mathbf{k} \in \mathcal{K}$,

1. *(Finite energy penalty of local flip) for some $\mathbf{G} \in \Gamma^*$,* $\operatorname{Im} \operatorname{Tr}\left(A_{\mathbf{k}}(\mathbf{G})\right) \neq 0$
2. *(No hidden invariant subspace) for all non-trivial orthogonal projectors Π (i.e. $\Pi \neq 0, I$), there exists a $\mathbf{G} \in \Gamma^*$ so that*

$$\|(I - \Pi) A_{\mathbf{k}}(\mathbf{G}) \Pi\| > 0$$

then FSD states are the only uniformly filled, translational invariant Slater determinant ground states of $\hat{H}_{FBI}$.

These conditions can be explicitly verified in TBG-2, TBG-4 etc.

(Becker, Lin, **KDS**, CMP 2025)

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- If $\exists P$ a minimizer of E_{HF} but not E_F, then contradiction:

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- The rest goes to prove FSD states are the only minimizers of E_F.

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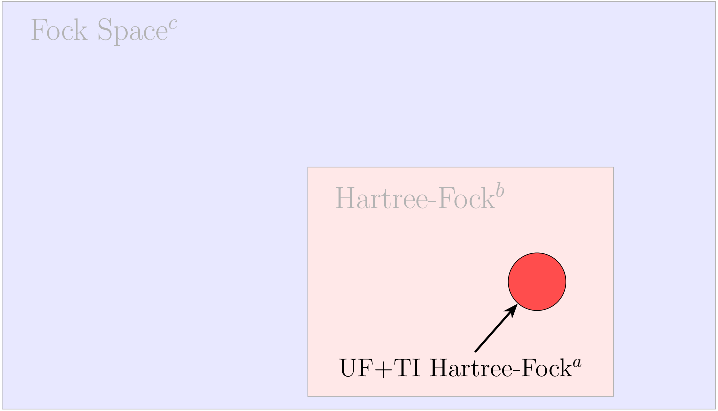

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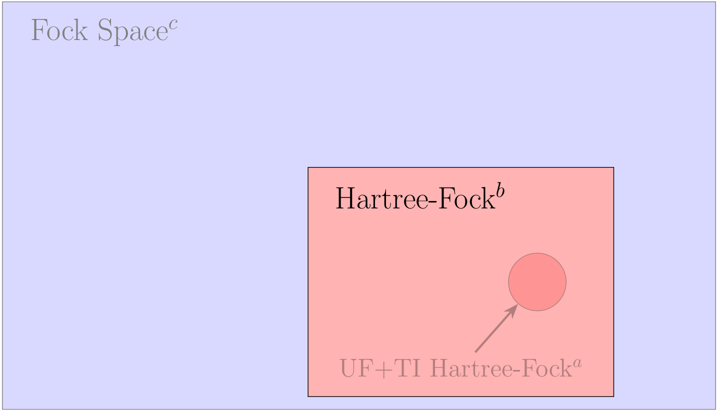

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Main Result for TBG-2

Theorem (Informal)

For TBG-2, Hartree-Fock ground state manifold of $\hat{H}_{\mathrm{FBI}}$ consists of:

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(**KDS**, Becker, Lin SIAM MMS 2025)

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- *(Spinless and Valleyful) Orbits of $\mathrm{U}(2) \times \mathrm{U}(2)$ on three elements.*

(**KDS**, Becker, Lin SIAM MMS 2025)

Main Result for TBG-2

Theorem (Informal)

For TBG-2, Hartree-Fock ground state manifold of $\hat{H}_{\mathrm{FBI}}$ consists of:

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- In TBG, there are two chiral sectors; $\mathrm{U}(2)$ or $\mathrm{U}(4)$ rotations are within each of the chiral sectors.

(**KDS**, Becker, Lin SIAM MMS 2025)

Optimality Conditions for 1-RDM

Theorem

If P is the 1-RDM of Hartree-Fock ground state of a frustration free FBI Hamiltonian if and only if for all $\mathbf{q} \in \mathcal{K}$ and all $\mathbf{G} \in \Gamma^*$:

$$\sum_{\mathbf{k}'' \in \mathcal{K}} \mathrm{Tr}\left(\Lambda_{\mathbf{k}''}(\mathbf{q}+\mathbf{G}) \left(P(\mathbf{k}''+\mathbf{q}, \mathbf{k}'') - \frac{1}{2}\delta_{\mathbf{q},\mathbf{0}} I \right) \right) = 0$$

and for all $\mathbf{k}, \mathbf{k}' \in \mathcal{K}$

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- Therefore $P(\mathbf{k}, \mathbf{k}') \neq 0$ if and only if for all $\mathbf{G} \in \Gamma^*$ $\Lambda_{\mathbf{k}}(\mathbf{G})$ and $\Lambda_{\mathbf{k}'}(\mathbf{G})$ share at least one eigenvalue.

Sylvester Equation in TBG-2

Proposition

For TBG-2, the family of Sylvester equations:

$$X\Lambda_{\mathbf{k}'}(\mathbf{G}) - \Lambda_{\mathbf{k}}(\mathbf{G})X = 0 \qquad \forall \mathbf{G} \in \Gamma^*$$

has a non-zero solution if and only if $\mathbf{k}' = \mathbf{k}$ *or* $\mathbf{k}' = -\mathbf{k}$.

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- For TBG-2, the matrices $\Lambda_{\mathbf{k}}(\mathbf{G})$ are diagonal and known semi-explicitly $\quad \Rightarrow \quad P(\mathbf{k}, \mathbf{k}') = 0$ for $\mathbf{k}' \neq -\mathbf{k}$.

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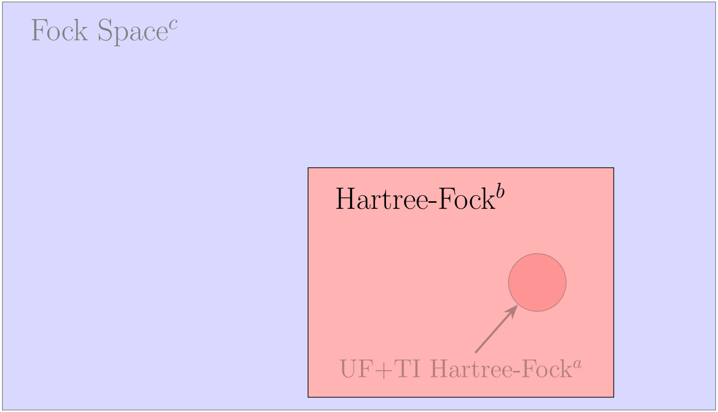
- Together with $P(\mathbf{k}, -\mathbf{k}) = 0$ for $\mathbf{k} \neq 0 \quad \Rightarrow \quad P(\mathbf{k}, \mathbf{k}') = P(\mathbf{k})\delta_{\mathbf{k},\mathbf{k}'}$
  $\Rightarrow \quad$ HF ground states are translation invariant.

Hierarchy of Admissible States



[a](Becker, Lin, **KDS** CMP 2025), [b](**KDS**, Becker, Lin, SIAM MMS 2025), [c](**KDS**, Ragone, MacDonald, Lin, arXiv: 2503.20060)

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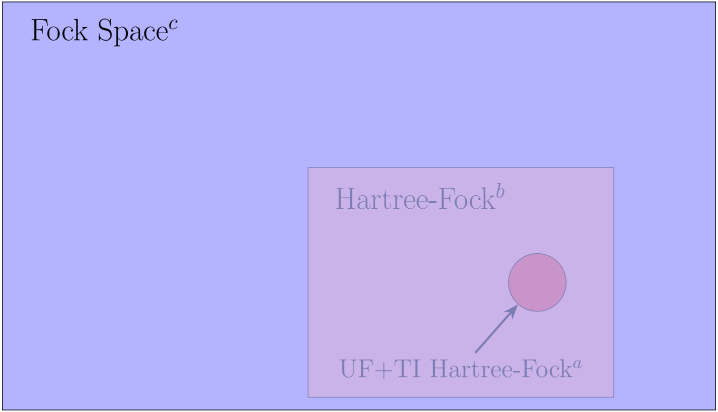

[a](Becker, Lin, **KDS** CMP 2025), [b](**KDS**, Becker, Lin, SIAM MMS 2025), [c](**KDS**, Ragone, MacDonald, Lin, arXiv: 2503.20060)

FBI Hamiltonian Revisited

$$\hat{H}_{FBI} = \frac{1}{N_{\mathbf{k}}|\mathbb{R}^2/\Gamma|} \sum_{\mathbf{q}' \in \mathcal{K}+\Gamma^*} \hat{V}(\mathbf{q}')\widehat{\rho}(\mathbf{q}')\widehat{\rho}(-\mathbf{q}')$$

- $|\Phi\rangle$ is a ground state if and only if

$$\hat{\rho}(\mathbf{q}')\,|\Phi\rangle = 0.$$

Constraints from $\widehat{\rho}(\mathrm{G})$

- When $\mathbf{q}' = \mathbf{G} \in \Gamma^*$

$$\widehat{\rho}(\mathbf{G}) = \sum_{\mathbf{k} \in \mathcal{K}} a_{\mathbf{k}}(\mathbf{G}) \Big(\hat{n}_{+,\mathbf{k}} + \hat{n}_{-,(-\mathbf{k})} - 4 \Big)$$

$\hat{n}_{+,\mathbf{k}}$, $\hat{n}_{-,\mathbf{k}}$: number operators for the two chiral sectors.

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$\hat{n}_{+,\mathbf{k}}$, $\hat{n}_{-,\mathbf{k}}$: number operators for the two chiral sectors.

- Ground state $|\Phi\rangle$ satisfies

$$\sum_{\mathbf{k}\in\mathcal{K}} a_{\mathbf{k}}(\mathbf{G})\Big(\hat{n}_{+,\mathbf{k}} + \hat{n}_{-,(-\mathbf{k})} - 4\Big)\,|\Phi\rangle = 0$$

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\sum_{\mathbf{k}\in\mathcal{K}} a_{\mathbf{k}}(\mathbf{G}_2)\left(\hat{n}_{+,\mathbf{k}} + \hat{n}_{-,(-\mathbf{k})} - 4\right)|\Phi\rangle &= 0 \\
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$$

- Fix an arbitrary state $|\tilde{\Phi}\rangle$ and define

$$
\nu_{\mathbf{k}} := \langle \tilde{\Phi}, \Big(\hat{n}_{+,\mathbf{k}} + \hat{n}_{-,(-\mathbf{k})} - 4\Big)\Phi\rangle
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\quad \Longrightarrow \quad
\begin{bmatrix}
a_{\mathbf{k}_1}(\mathbf{G}_1) & \cdots & a_{\mathbf{k}_{N_{\mathbf{k}}}}(\mathbf{G}_1) \\
a_{\mathbf{k}_1}(\mathbf{G}_2) & \cdots & a_{\mathbf{k}_{N_{\mathbf{k}}}}(\mathbf{G}_2) \\
\vdots & \ddots & \vdots
\end{bmatrix} \nu = 0
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“Hidden Conservation Law” for ground states

Lemma

For all finite sets $\mathcal{K} \subseteq \mathbb{R}^2/\Gamma^*$,

$$\ker\left(\begin{bmatrix} a_{\mathbf{k}_1}(\mathbf{G}_1) & \cdots & a_{\mathbf{k}_{N_\mathbf{k}}}(\mathbf{G}_1) \\ a_{\mathbf{k}_1}(\mathbf{G}_2) & \cdots & a_{\mathbf{k}_{N_\mathbf{k}}}(\mathbf{G}_2) \\ \vdots & \ddots & \vdots \end{bmatrix}\right) = \{\mathbf{0}\}$$

Corollary

If $|\Phi\rangle$ is a ground state, then for all $\mathbf{k}$ it satisfies

$$\left(\hat{n}_{+,\mathbf{k}} + \hat{n}_{-,(-\mathbf{k})} - 4\right)|\Phi\rangle = 0$$

Constraints on number of electrons at each $\mathbf{k}$.
Many-body generalization of constraints from Sylvester equations.

Characterization of the Many-Body Ground States

Proposition (Uniform filling)

$$|\Phi_{GS}\rangle = \sum_{n_+=0}^{4} c_{n_+} |\Phi_{n_+}\rangle$$

where $|\Phi_{n_+}\rangle$ has n_+ electrons in the $+$ sector at every $\mathbf{k}$.

Characterization of the Many-Body Ground States

- Two chiral sectors $+$, $-$.

Creation for $+$: $\hat{f}^\dagger_{(+,+,\uparrow),\mathbf{k}}$ $\hat{f}^\dagger_{(+,+,\downarrow),\mathbf{k}}$ $\hat{f}^\dagger_{(-,-,\uparrow),\mathbf{k}}$ $\hat{f}^\dagger_{(-,-,\downarrow),\mathbf{k}}$

Creation for $-$: $\hat{f}^\dagger_{(+,-,\uparrow),\mathbf{k}}$ $\hat{f}^\dagger_{(+,-,\downarrow),\mathbf{k}}$ $\hat{f}^\dagger_{(-,+,\uparrow),\mathbf{k}}$ $\hat{f}^\dagger_{(-,+,\downarrow),\mathbf{k}}$

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- Relabel creation operators with $1^\pm, 2^\pm, 3^\pm, 4^\pm$

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- One possible choice for $|\Phi_{n_+=1}\rangle$

$$\left(\prod_{\mathbf{k}} \hat{f}^{\dagger}_{1^+,\mathbf{k}}\right)\left(\prod_{\mathbf{k}} \hat{f}^{\dagger}_{1^-,\mathbf{k}}\hat{f}^{\dagger}_{2^-,\mathbf{k}}\hat{f}^{\dagger}_{3^-,\mathbf{k}}\right)|\text{vac}\rangle$$

Characterization of the Many-Body Ground States

- For any $U \in \mathrm{U}(4)$ define

$$U \circ \hat{f}^{\dagger}_{1+,\mathbf{k}} = u_{11}\hat{f}^{\dagger}_{1+,\mathbf{k}} + u_{21}\hat{f}^{\dagger}_{2+,\mathbf{k}} + u_{31}\hat{f}^{\dagger}_{3+,\mathbf{k}} + u_{41}\hat{f}^{\dagger}_{4+,\mathbf{k}}$$

which rotates creation operators by U within $+$ sector.

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- Define $U \circ \hat{f}^{\dagger}_{1-,\mathbf{k}}\hat{f}^{\dagger}_{2-,\mathbf{k}}\hat{f}^{\dagger}_{3-,\mathbf{k}}$ by rotating each creation operator.

- Can show for any $U, V \in \mathrm{U}(4)$ all states of the form

$$\left(\prod_{\mathbf{k}} U \circ \hat{f}^{\dagger}_{1+,\mathbf{k}}\right)\left(\prod_{\mathbf{k}} V \circ \hat{f}^{\dagger}_{1-,\mathbf{k}}\hat{f}^{\dagger}_{2-,\mathbf{k}}\hat{f}^{\dagger}_{3-,\mathbf{k}}\right)|\text{vac}\rangle$$

have the same energy $\Rightarrow$ Study irreps of $\mathrm{U}(4) \times \mathrm{U}(4)$.

Occupation Representation and Young Diagrams

$$(\mathbb{C}^4)^{\otimes N_{\mathbf{k}}} \qquad\qquad (\mathbb{C}^4 \wedge \mathbb{C}^4 \wedge \mathbb{C}^4)^{\otimes N_{\mathbf{k}}}$$

$$\bigcup \qquad\qquad\qquad\qquad \bigcup$$

$$\underbrace{\square\square\square\square\square\square\square}_{N_{\mathbf{k}}} \qquad\qquad \underbrace{\begin{array}{ccccccc} \square&\square&\square&\square&\square&\square&\square \\ \square&\square&\square&\square&\square&\square&\square \\ \square&\square&\square&\square&\square&\square&\square \end{array}}_{N_{\mathbf{k}}}$$

$$\left(\prod_{\mathbf{k}} U \circ \hat{f}^{\dagger}_{1+,\mathbf{k}}\right) \quad \left(\prod_{\mathbf{k}} V \circ \hat{f}^{\dagger}_{1-,\mathbf{k}}\hat{f}^{\dagger}_{2-,\mathbf{k}}\hat{f}^{\dagger}_{3-,\mathbf{k}}\right) |\text{vac}\rangle$$

- $U, V \in \mathrm{U}(4)$.
- Horizontal: symmetrization; Vertical: anti-symmetrization

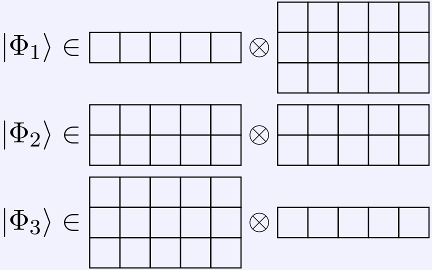
Many-Body Ground States

Theorem

Any many-body ground state for spinful, valleyful chiral TBG:

$$\alpha_0 \left|\Phi_0\right\rangle + \alpha_1 \left|\Phi_1\right\rangle + \alpha_2 \left|\Phi_2\right\rangle + \alpha_3 \left|\Phi_3\right\rangle + \alpha_4 \left|\Phi_4\right\rangle$$

where $\left|\Phi_4\right\rangle$ *and* $\left|\Phi_0\right\rangle$ *fully fill the* $+$ *and* $-$ *sector respectively and*



Inductive proof showing all other diagrams have positive energies.
Hook length formula gives dimension counting of the manifold.
(**KDS**, Ragone, MacDonald, Lin, arXiv: 2503.20060)

Outline

Relaxed Bistritzer-MacDonald Model

- Complete characterization of ground states of TBG for Bistritzer-MacDonald (BM) model at chiral limit.

(Quinn, Kong, Luskin, Watson JMP 2025), see also (Kang, Vafek PRB 2023)

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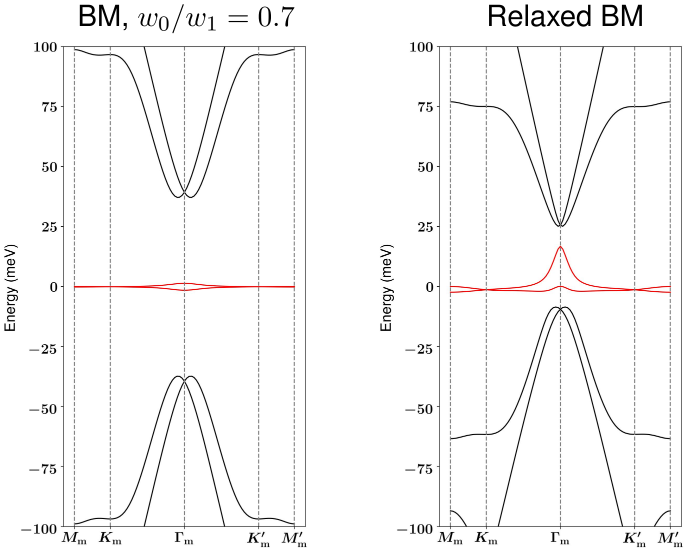
- Relaxation and hopping parameters determined from DFT.

(Quinn, Kong, Luskin, Watson JMP 2025), see also (Kang, Vafek PRB 2023)

Single Particle Band Structure

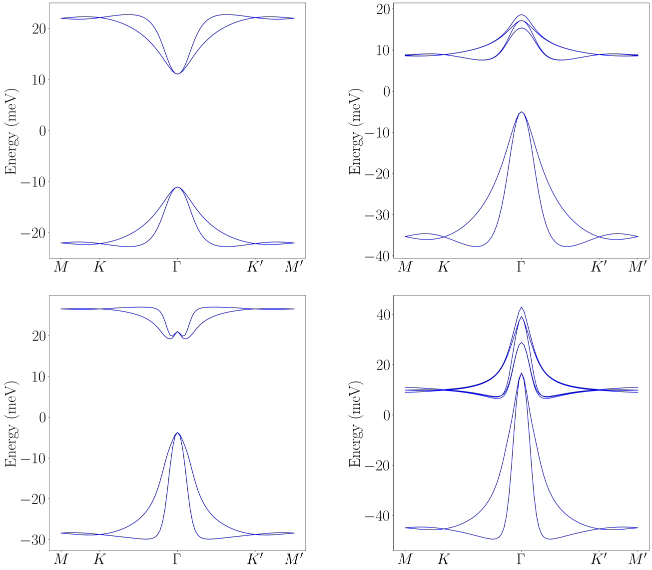


Hartree-Fock Band Structure

$\nu = 0$ $\nu = -2$

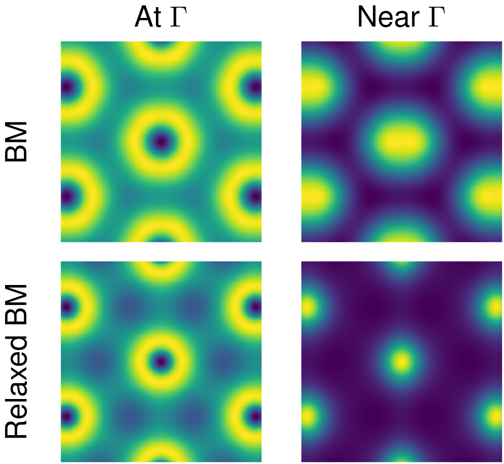
BM, $w_0/w_1 = 0.7$

Relaxed BM



Why Metallic Behavior?

- Most likely culprit (below, plot of $\sum_n |\psi_{n\mathbf{k}}(\mathbf{r})|^2$):



Outline

Discussion

- What do the low energy excitations look like in chiral TBG? Can we rigorously characterize them?
- Extension of ground state result to other models (cf. vortexability)?
- Why do eigenfunctions concentrate in relaxed BM?
- Experimentally, strain is known to be very important. What happens with realistic strain?

Acknowledgments

Thank you for your attention!

Kevin Stubbs
https://kstub.github.io

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